

6-Methyl-3-(2-nitroxyethyl)-2H-1,3-benzoxazin-4(3H)-one

Other names:	2,3-Dihydro-6-methyl-3-[2-(nitrooxy)ethyl]-4H-1,3-benzoxazin-4-one
Inchi:	InChI=1S/C11H12N2O5/c1-8-2-3-10-9(6-8)11(14)12(7-17-10)4-5-18-13(15)16/h2-3,6H,4
InchiKey:	PRQKFPKMNWUHSR-UHFFFAOYSA-N
Formula:	C11H12N2O5
SMILES:	<chem>Cc1ccc2c(c1)C(=O)N(CCO[N+](=O)[O-])CO2</chem>
Mol. weight [g/mol]:	252.22
CAS:	143248-64-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	0.995		Crippen Method
mcvol	171.940	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.10	kJ/mol	351.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C143248640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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